Iterative solution of differential equations

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Abstract

We discuss alternative iteration methods for differential equations. We provide a convergence proof for exactly solvable examples and show more convenient formulas for nontrivial problems.

1 Introduction

The asymptotic iteration method (AIM) is an algorithm for the exact and approximate solution of second–order ordinary differential equations [1, 2].

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It has been applied to a wide variety of problems that include exact and approximate calculations of eigenvalues and eigenfunctions, implementation of perturbation theory, nonrelativistic and relativistic problems, among others [3–11].

Almost all those references are devoted to applications of the approach and little has been done to provide a sound foundation for the AIM. The proofs given in the first two papers on the subject [1, 2] do not account for all the properties of the method. Recently, Matamala et al derived a most interesting connection between the AIM and continued fractions [12].

The purpose of this paper is to provide a deeper insight into the AIM. In Sec. 2 we give well known formal solutions to the differential equation. In Sec. 3 we discuss the AIM and some conditions for its successful application to exactly solvable and nontrivial problems. We discuss a simple problem with constant coefficients in order to illustrate the kind of solutions expected from the AIM. In Sec. 4 we propose alternative iterative approaches that we apply to the same simple problem just mentioned. In Sec. 5 we apply the AIM to the harmonic and anharmonic oscillators, compare alternative recurrence relations and the effect of different initial conditions. Finally we summarize our results and draw conclusions in Sec. 6.

2 Differential equation

The purpose of this paper is the exact or approximate solution of differential equations of the form

$$y''(x) = p(x)y'(x) + q(x)y(x) \tag{1}$$

where $p(x)$ and $q(x)$ are integrable functions. We can easily obtain a formal solution to this equation if we factorize it as

$$\left[\frac{d}{dx}+a(x)\right]\left[\frac{d}{dx}+b(x)\right]y(x)=0. \tag{2}$$

On comparing both equations we realize that $a(x)=-p(x)-b(x)$ where $b(x)$ is a solution of the Riccati equation

$$b'(x)-b(x)^2-p(x)b(x)+q(x)=0. \tag{3}$$

Straightforward integration of equation (2) yields the general solution

$$y(x)=\exp\left[-\int^{x}b(u)\,du\right]\left\{C_1+C_2\int^{x}\exp\left[\int^{t}(2b(u)+p(u))\,du\right]dt\right\} \tag{4}$$

where C_1 and C_2 are integration constants. Notice that it is a linear combination of two independent solutions of Eq. (1).

The logarithmic derivative

$$f(x)=-\frac{y'(x)}{y(x)} \tag{5}$$

also satisfies the Riccati equation (3):

$$f'(x)-f(x)^2-p(x)f(x)+q(x)=0. \tag{6}$$

All those results are well known, and we summarize them here merely to facilitate the discussion below.

3 Asymptotic Iteration Method

The AIM is applicable if $p(x)$ and $q(x)$ are C^{∞} functions. If we differentiate Eq. (1) n times we obtain

$$y^{(n+2)}(x) = p_n(x)y'(x) + q_n y(x) \tag{7}$$

where

$$\begin{aligned} p_n &= p'_{n-1} + pp_{n-1} + q_{n-1}, \\ q_n &= q'_{n-1} + qp_{n-1},\ n = 1, 2, \dots \\ p_0 &= p,\ q_0 = q. \end{aligned} \tag{8}$$

Ciftci et al [1] proved that if

$$\frac{q_n}{p_n} = \frac{q_{n-1}}{p_{n-1}} = \alpha \tag{9}$$

then

$$y(x) = \exp\left[-\int^{x} \alpha(u)\, du\right] \left\{C_1 + C_2 \int^{x} \exp\left[\int^{t} (2\alpha(u) + p(u))\, du\right] dt\right\}. \tag{10}$$

is a general solution of the differential equation (1). It is clear that Eq. (10) agrees with Eq. (4) if $\alpha(x) = b(x)$ [2] and its existence is therefore independent of the condition (9). Moreover, we conclude that $\alpha(x)$ should satisfy the Riccati equation (3).

Saad et al [13] proved that the exact solutions just discussed are polynomial functions. In what follows we provide an alternative proof that is more convenient for the treatment of nontrivial problems. If we differentiate the ratio q_{n-1}/p_{n-1} and use the recurrence relations (8) we obtain

$$\left(\frac{q_{n-1}}{p_{n-1}}\right)' - \left(\frac{q_{n-1}}{p_{n-1}}\right)^2 - p\frac{q_{n-1}}{p_{n-1}} + q = \frac{\delta_n}{p_{n-1}^2}. \tag{11}$$

where

$$\delta_n = q_n p_{n-1} - q_{n-1} p_n. \tag{12}$$

Therefore, if $\delta_n = 0$ and $p_{n-1} \neq 0$ then $\alpha = q_{n-1}/p_{n-1}$ satisfies the Riccati equation (3) and $y = C \exp\left[-\int^x \alpha(u)\, du\right]$ is a solution to the differential equation (1). Since $y^{(n+1)} = p_{n-1}(y' + \alpha y) = 0$ we conclude that $y(x)$ is polynomial of degree at most n . Conversely, if $y(x)$ is a polynomial solution of degree n, then $y' + q_{n-1}y/p_{n-1} = 0$, provided that $p_{n-1} \neq 0$, $\alpha = q_{n-1}/p_{n-1}$ satisfies the Riccati equation and $\delta_n = 0$. Summarizing, there is a polynomial solution $y(x)$ to Eq. (1) if and only if $\delta_n = 0$ and $p_{n-1} \neq 0$. This is exactly theorem 2 of reference [13] except that present proof does do not require that $p_n \neq 0$. One can easily verify that if $p_n = 0$ then $q_k = p_k = 0$ for all $k \geq n$ under the conditions above.

The condition (9), although useful for exactly solvable problems, is not suitable for nontrivial ones where we require that

$$\lim_{n\to\infty} \frac{q_n}{p_n} = \alpha. \tag{13}$$

Notice that if

$$\lim_{n\to\infty} \frac{\delta_n}{p_{n-1}^2} = 0 \tag{14}$$

then $\alpha(x)$ given by Eq. (13) is a solution of the Riccati equation (3) and Eq. (10) is the general solution of the differential equation (1).

In order to understand some of the main features of the AIM it is convenient to discuss a simple problem already considered earlier. If $p(x)$ and $q(x)$ are constant, then the AIM recurrence relations (8) are exactly solvable:

$$\begin{aligned} p_n &= C_1 \rho_1^n + C_2 \rho_2^n, \\ q_n &= q p_{n-1}, \end{aligned}$$

$$\rho_{1,2} = \frac{p \pm \Delta}{2},\ \Delta = \sqrt{p^2 + 4q}, \tag{15}$$

where the constants C_1 and C_2 are determined by the conditions $p_0 = p$ and $p_{-1} = 1$.

If $|\rho_1| < |\rho_2|$ equation (13) gives us $\alpha = -\rho_1$ that is a root of the Riccati equation (3) ($b'(x) = 0$). We appreciate that the AIM yields the root with smaller modulus and we then obtain the general solution by means of Eq. (10). This extremely simple exactly solvable example is interesting because its solutions are not polynomials.

If $|\rho_1| = |\rho_2|$ and $\rho_1 \neq \rho_2$ the AIM does not converge but we can overcome this difficulty quite easily. The function $v(x) = y(x)\exp(\beta x)$ is a solution of the differential equation $v''(x) = \tilde{p}v'(x) + \tilde{q}v(x)$, where $\tilde{p} = 2\beta + p$ and $\tilde{q} = q - p\beta - \beta^2$. The new roots are $\tilde{\rho}_{1,2} = \beta + \rho_{1,2}$ and the AIM converges for the modified differential equation because $|\tilde{\rho}_1| \neq |\tilde{\rho}_2|$. We will see that transformations of this sort are useful for the treatment of the Schrödinger equation. Clearly, this strategy fails when $\rho_1 = \rho_2$.

4 Iterative Riccati method

It is clear from the discussion above that the Riccati equation (6) is central to the AIM. We can derive the AIM from the Riccati equation if we look for a solution of the form

$$f(x) = \frac{A(x)}{B(x)}. \tag{16}$$

On substituting this expression into the Riccati equation and rearranging conveniently we obtain [2]

$$\frac{A}{B} = \frac{A' + qB}{B' + A + pB}. \tag{17}$$

If we solve the equations $A = A' + qB$, and $B = B' + A + pB$ iteratively we obtain the AIM recurrence relations

$$\begin{aligned} A_n &= A'_{n-1} + qB_{n-1}, \\ B_n &= B'_{n-1} + A_{n-1} + pB_{n-1}, \end{aligned} \tag{18}$$

except that we do not have any prescription for the initial conditions A_0 and B_0. However, according to the example of the preceding section, the initial conditions do not appear to be that relevant for nonpolynomial solutions. The most important fact is that

$$\left(\frac{A_{n-1}}{B_{n-1}}\right)' - \left(\frac{A_{n-1}}{B_{n-1}}\right)^2 - p\frac{A_{n-1}}{B_{n-1}} + q = \frac{\delta_n}{B_{n-1}^2} \tag{19}$$

where $\delta_n = B_{n-1}A_n - B_nA_{n-1}$, which clearly tell us that the sequence of ratios A_{n-1}/B_{n-1} may converge to a solution of the Riccati equation.

We can rearrange the equation for A and B in a different way

$$\frac{A}{B} = \frac{A' - pA + qB}{B' + A} \tag{20}$$

and derive the alternative recurrence relations

$$\begin{aligned} A_n &= A'_{n-1} - pA_{n-1} + qB_{n-1} \\ B_n &= B'_{n-1} + A_{n-1}. \end{aligned} \tag{21}$$

This approach does not agree with the AIM. We appreciate that the iterative Riccati method is somewhat more arbitrary than the AIM.

The sequences $\{A_n^{(1)}, B_n^{(1)}\}$ and $\{A_n^{(2)}, B_n^{(2)}\}$ given by the recurrence relations (18) and (21), respectively, are not independent. In fact, it is not difficult to prove that $A_n^{(2)}(x) = A_n^{(1)}(x)e^{u(x)}$, and $B_n^{(2)}(x) = B_n^{(1)}(x)e^{u(x)}$, where $u'(x) = p(x)$. Both recurrence relations should give the same result if the initial conditions are also related by the same transformation.

If we apply equations (18) to the exactly solvable example discussed above we obtain the AIM result. On the other hand, if we apply equations (21) the result is the root of the Riccati equation with greater modulus: $\lim_{n\to\infty}(A_n/B_n) = \rho_2$. In both cases we assume $A_0' = B_0' = 0$.

5 The Schrödinger equation

Direct application of the AIM to the Schrödinger equation

$$\psi''(x) = [V(x) - E]\,\psi(x) \tag{22}$$

may lead to divergent sequences for nonpolynomial solutions. Notice that we meet the same difficulty when we apply the AIM to the simple example above with $p = 0$. In order to overcome it we make the transformation $\psi(x) = g(x)y(x)$ and apply the AIM to the resulting differential equation for $y(x)$:

$$y'' = -2\frac{g'}{g}y' + \left(V - E - \frac{g''}{g}\right)y. \tag{23}$$

It has been shown that the rate of convergence of the AIM sequences depends on the function $g(x)$ [2]. For example, in the case of the harmonic oscillator $V(x) = x^2$ we choose $g(x) = \exp(-x^2/2)$ and $y(x)$ satisfies the Hermite differential equation that we discuss briefly below. Notice that in the case of eigenvalue problems one has to determine the value of the energy E together with the solution $y(x)$. We obtain the eigenvalues E from the roots of $\delta_n = 0$. In the case of polynomial solutions this equation yields exact eigenvalues for finite n, but for nontrivial problems we obtain increasingly accurate results as $n \to \infty$. [1,2]

In order to have a deeper insight into the approaches derived above it is convenient to consider a simple differential equation with variable coefficients $p(x)$

and $q(x)$. One of the simplest examples is the Hermite differential equation [14]

$$y''(x) = 2xy'(x) - 2my(x) \tag{24}$$

with polynomial solutions for $m = 0, 1, \ldots$. This example is different from the preceding one in that the iteration method determines the value of m and, consequently, of q together with the solutions of the corresponding Riccati equation.

The terminating condition yields the values of m corresponding to the Hermite polynomials as shown by:

$$\begin{aligned} &\delta_n = -2^{n+1} m(m-1)\ldots(m-n) = 0. \\ &n = 1, 2, \ldots \end{aligned} \tag{25}$$

Besides, each of the functions

$$\begin{aligned} &m = 0 \Rightarrow \frac{A_n}{B_n} = 0, \; n \geq 0 \\ &m = 1 \Rightarrow \frac{A_n}{B_n} = -\frac{1}{x}, \; n \geq 0 \\ &m = 2 \Rightarrow \frac{A_n}{B_n} = -\frac{4x}{2x^2 - 1}, \; n \geq 1 \\ &m = 3 \Rightarrow \frac{A_n}{B_n} = -\frac{3(2x^2 - 1)}{x(2x^2 - 3)}, \; n \geq 2 \\ &\quad \ldots \end{aligned} \tag{26}$$

satisfies the Riccati equation with the corresponding value of $q = -2m$. In this case we have chosen the AIM initial conditions $A_0 = q$, and $B_0 = p$. Notice that given the value of m we obtain the exact polynomial solution from A_n/B_n for any $n \geq m - 1$.

If, on the other hand, we choose, for example, $A_0 = B_0 = 1$, then, for a given m we obtain the corresponding Hermite polynomial for all $n \geq m + 1$. That is to say, we need more iterations for the same result, which suggests that the AIM prescription is most convenient for this case.

As suggested by the simple example in Sec. 3 the alternative recurrence relation (21) may yield other kind of solutions. We have confirmed this point in the case of the Hermite equation. The roots of $\delta_n = 0$ are negative integers $m = -1, -2, \ldots$, and $A_n/B_n = -2x,\ -(1+2x^2)/x, \ldots$ for sufficiently large but finite n are solutions to the corresponding Riccati equation.

However, if we choose the initial conditions $A_0(x) = q(x)e^{x^2}$, and $B_0 = p(x)e^{x^2}$ in the recurrence relations (21), then we obtain exactly the AIM results in complete accordance with the discussion in Sec. 4.

As a nontrivial model we consider the anharmonic oscillator $V(x) = x^4$. We follow an earlier application of the AIM and choose $g(x) = \exp(\beta x^2/2)$ where β is an adjustable parameter [2]. However, in this case we select the initial conditions $A_0 = 1$ and $B_0 = 1$ arbitrarily for the recurrence relations (18).

Results are similar to those given by the standard AIM [2] which shows that the initial conditions are not so relevant in the case of nonpolynomial problems. Particularly, if a great number of iterations is required as in the present application.

6 Conclusions

In this paper we try to provide an alternative proof for the AIM in the case of exactly solvable examples and develop equations that appear to be more convenient for the discussion of nontrivial problems. We also expect to place the AIM in a more general context of iterative algorithms for differential equations as Matamala et al have also done regarding the continued fractions algorithm [12].

Present results suggest that the AIM gives a convenient prescription for the starting point of the recurrence relations if one is looking for the square inte-

grable solutions of the Schrödinger equation. However, other initial conditions may lead to identical results, particularly in the case of nonpolynomial problems where a great number of iterations is necessary for accurate results.

One can derive alternative recurrence relations that also give solutions to the Riccati equation and, consequently, to the linear differential equation. However, those alternative recurrence relations require that one chooses the initial conditions carefully; otherwise one may obtain unwanted solutions.

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